On Scale Determination in Lattice QCD with Dynamical Quarks

arXiv:0803.1281 [hep-lat]

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Simulations of Lattice QCD with dynamical quarks show:

Sommer parameter $r_c/a$ depends on sea quark mass $am_q$.

The Questions are

- Is this a cut-off effect or a physical effect?
- How is the lattice scale to be determined?
  - Should the scale $a$ be taken as dependent on the quark mass $m_q$?
  - Since the quark mass is a scale-dependent quantity, how to do chiral extrapolations of hadronic quantities like masses?

NO theoretical understanding yet!
Our Simulation

- Wilson (unimproved) gauge and fermion actions (\(\mathcal{O}(a)\) cutoff effects)
- \(N_F = 2\) degenerate sea quarks
- \(\beta = 6/g^2 = 5.6\), 16\(^3\)32 lattice
- 8 values of sea quark masses, \(am_q \approx 0.07 - 0.014\)

- Standard HMC updating so far (DDHMC runs in progress)
- 5000 trajectories at each sea quark mass
- Gaussian smearing at both mesonic source and sink, highly optimized, arXiv:0712.4354 [hep-lat]
- APE smearing used to extract static potential from \(<W>\)

- All errors shown are single-omission JK errors from 200 independent configurations at each quark mass
Analysis of $\langle W(R, T) \rangle$

- Smearing level up to 40 with $\epsilon = 2.5$ where $c/4 = 1/(\epsilon + 4)$ is the coefficient of the staples

- $\langle W(R, T) \rangle$ measured up to $T = 16$ and $R = 8\sqrt{3}$

- Reasonable plateau obtained in effective potential plots between $T = 3$ and $T = 5$

- Static potential $V(R)$ extracted from single exponential fits between $[T_{min}, T_{max}] = [3, 4]$, $[3, 5]$, $[4, 5]$

  $$\langle W(R, T) \rangle = C(R) \exp[-aV(R)T]$$

- Optimum smearing level determined at a given quark mass by observing the ground state overlap $C(R)$ as a function of $R$
$\beta = 5.6, \kappa = 0.15775 \ (am_q \approx 0.02)$
Analysis of $aV(R)$

At each $\beta$ and quark mass, the static potential obtained is analyzed with the following parameterization:

$$aV(R) = aV_0 + a^2\sigma R - \frac{\alpha}{R} - \delta_{\text{ROT}} \left( \left[ \frac{1}{R} \right] - \frac{1}{R} \right)$$

where $\delta_{\text{ROT}}$ is the coeff of the lattice correction term with

$$\left[ \frac{1}{R} \right] = \frac{4\pi}{L^3} \sum_{q_i \neq 0} \frac{\cos(aq_i \cdot R)}{4\sin^2(aq_i/2)}$$

being the lattice fourier transform of the gluon propagator.

The first 3 terms of $aV(R)$ above is differentiated to obtain the Sommer parameter: $a/r_c = 1/R_c = a\sigma^{1/2}/\sqrt{(N_c - \alpha)}$
\[ \beta = 5.6, \quad \kappa = 0.1575 \quad (a m_q \approx 0.03) \]

- The difference \([1/R - 1/R]\) is never negligible on a finite lattice.
- \(\alpha\) is expected to run with \(R\) at these intermediate length scales.
- Can only estimate an average \(\alpha\) over the values of \(R\) where the static potential is fit.
- Perturbative running is generally applicable at scales \(\gtrsim 2 \text{ GeV}\) which translates into \(R \lesssim 1\) in our case.
\[ \beta = 5.6, \kappa = 0.1575 \]
\[ (am_q \approx 0.03) \]
The Problem

Simulation

Results

Scale Determination

Conclusion

\[ \beta = 5.6 \]

\[ \alpha = 0.3 \]

\[ aV_0 \]

\[ \delta_{\text{ROT}} \]

\[ a\sigma_{1/2} \]
$\beta = 5.6$
From the numerical results on $\alpha$, $a\sigma^{1/2}$ and $a/r_c$ in dependence of $am_q$, at fixed $\beta$, we conclude:

- The dimensionless parameter $\alpha$ does NOT significantly depend on $am_q$ for small enough $am_q$ ($\lesssim 0.035$).
- Scaling violations (= cutoff effects) are negligible for small enough $am_q$.
- $a\sigma^{1/2}$ is linear in $am_q$ for small enough $am_q$:
  \[ a\sigma^{1/2} = C_1 + C_2 am_q \]
- $a/r_c$ is linear in $am_q$ for small enough $am_q$:
  \[ a/r_c = A_c + B_c am_q \]
- The qualitative content of the above conclusions does NOT change with any sensible change of the parameters of the analysis like $T_{min}$, $T_{max}$, $R_{min}$, $R_{max}$ and the smearing level.
Check with a different

\( R_{\text{min}} = 2.0 \)

\( \beta = 5.6 \)
\[ \beta = 5.6 \]

- \( a/r_c \) is relatively independent of the choice of \( R_{min} \)
- For our final analysis, we settled for APE smearing level = 30 (for the lightest 3 quark masses) and 25 for the rest of the quark masses

\[
[T_{min}, T_{max}] = [3, 4] \\
[R_{min}, R_{max}] = [\sqrt{2}, 3\sqrt{5}]
\]
We interpret our results at fixed $\beta$ for small $am_q \lesssim 0.035$:

- $\alpha$ independent of $am_q$
- $a\sigma^{1/2} = C_1 + C_2 am_q$
- $a/r_c = A_c + B_c am_q$

To be a physical dependence of $\sigma^{1/2}$ and $1/r_c$ on $m_q$:

- $\sigma^{1/2} = C_1 + C_2 m_q$ with $C_1 = aC_1$
- $1/r_c = A_c + B_c m_q$ with $A_c = aA_c$

In other words, for data points with small enough $am_q$, at fixed $\beta$, the scale is taken to be the same for all quark masses $\Rightarrow$ a mass-independent scheme and a valid linear chiral extrapolation of $a/r_c$ and $a\sigma^{1/2}$ in the small $am_q$ region.
For chiral extrapolation of $a/r_c$ to the physical point, use dependence on $(am_\pi)^2$, instead of $(r_cm_\pi)^2$ or $(m_\pi/m_\rho)^2$:

$$a/r_c = P_c + Q_c(am_\pi)^2$$

Obtain the scale $a$ by solving the quadratic equation in $a$:

$$\frac{a}{r_c^{\text{Ph}}} = P_c + Q_c(am_\pi^{\text{Ph}})^2$$

where $r_c^{\text{Ph}}$ and $am_\pi^{\text{Ph}}$ are the physical values in physical units

Check chiral limits with $am_q$ and $(am_\pi)^2$ extrapolations:

<table>
<thead>
<tr>
<th>Extrapolation</th>
<th>Chiral limit of $a/r_0$</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$am_\pi$ from PP</td>
</tr>
<tr>
<td></td>
<td>$am_q^{\text{AA}}$</td>
</tr>
<tr>
<td>$am_q$</td>
<td>0.1616(13)</td>
</tr>
<tr>
<td>$(am_\pi)^2$</td>
<td>0.1631(16)</td>
</tr>
</tbody>
</table>
Our fit (right) drops the lowest \((am_\pi)^2\) points for FS effects and also drops some of the largest mass points for possible scaling violation.

Below is shown a similar plot from CPPACS (2002).
### The scale $a$ and $a^{-1}$

<table>
<thead>
<tr>
<th></th>
<th>$a m_\pi$ from PP</th>
<th></th>
<th>$a m_\pi$ from AA</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$a$ (fm) $a^{-1}$ (GeV)</td>
<td>$a$ (fm) $a^{-1}$ (GeV)</td>
<td></td>
</tr>
<tr>
<td>$a/r_0$ fit</td>
<td>0.08027(77) 2.458(23)</td>
<td>0.08032(76) 2.457(23)</td>
<td></td>
</tr>
<tr>
<td>$a/r_1$ fit</td>
<td>0.08053(70) 2.450(21)</td>
<td>0.08053(71) 2.450(22)</td>
<td></td>
</tr>
</tbody>
</table>

Contrast that with our own fully hadronic scale determination from linear dependence of $am_\rho$ on $(am_\pi)^2$: $am_\rho = F_1 + F_2 (am_\pi)^2$

| $am_\rho$ fit | 0.07932(135) 2.488(41) | 0.07995(195) 2.468(60) |
Concluding Remarks

The Problem

- All lattice actions (including all improved gauge and fermion actions) have shown the Sommer parameter in lattice units ($r_c/a$) depends on the sea quark mass in lattice units ($am_q$)
- All of this dependence then cannot be a scaling violation (positive power of the scale $a$). It must partly be a physical effect (see McNeile and Bernard et al, Lattice 2007)
- How to get rid of the scale-violating part?

Our simulation

- Our approach was to take Wilson action with $\mathcal{O}(a)$ effects and investigate the quark mass dependence at as many small enough quark masses as possible (8 values $\sim 0.014$ to 0.07) at a small enough lattice spacing (0.08 fm)
Importance of $\alpha$

- Essential to determine $\alpha$, the coeff of the $1/R$ term as carefully as possible. Its behavior with respect to changes of smearing level and $R_{\text{min}}$ should come out as expected.

Our Interpretation

- The dimensionless $\alpha$ being independent of $am_q$ for small $am_q$ is interpreted as a signal for getting rid of the scale-violating region.

- For the same range of $am_q$, $a\sigma^{1/2}$ and $a/r_c$ are both linear in $am_q$. This is interpreted as physical linear $m_q$ dependence of $\sigma^{1/2}$ and $1/r_C$, all in physical units.

- For our $\beta$ (=5.6), this region of quark mass is approximately $m_q < 85$ MeV
Chiral Extrapolation

- With the basic premises set, accurate chiral extrapolation needed to determine the lattice scale
  - Have used \((am_\pi)^2\) for extrapolation to the physical point
  - Only linear extrapolation in \((am_\pi)^2\) is done only for small masses (generally consistent with \(am_q < 0.035\)). Larger masses show deviation from linear behavior and in our experience these are scaling violations and should NOT be included in the fit.
  - Have checked the chiral limit with \(am_q\) extrapolation
  - Extrapolations with \((r_cm_\pi)^2\) and \((m_\pi/m_\rho)^2\) are better avoided. Introduce uncertainty and inaccuracy.
  - The whole procedure is testable with larger volumes and smaller quark masses (simulations underway with DDHMC)